



Training Services

Hydrocarbon Properties

IPD-2004/HCP1-1

Sources of Information About Hydrocarbon Properties

- Text books or handbooks
- Academic publications
- Trade journals
- Refinery laboratory data

IPD-2004/HCP1-2

Typical Properties of Hydrocarbons Determined in Laboratory

- Composition by chromatography
- ASTM distillations, simulated distillation
- Density or API gravity
- Hydrocarbon type as paraffin, olefin, naphthenes, and/or aromatics
- Viscosity
- RON and MON, smoke point, cetane number
- Cold flow properties - cloud point, pour point, freeze point
- Flash points
- Sulfur, nitrogen, Conradson Carbon, metals

IPD-2004/HCP1-3

RON — Research Octane
MON — ~~Motor~~ ~~Motor~~ ~~Motor~~ Octane

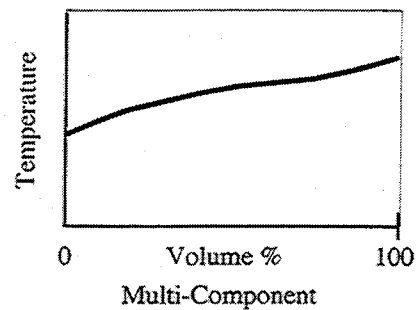
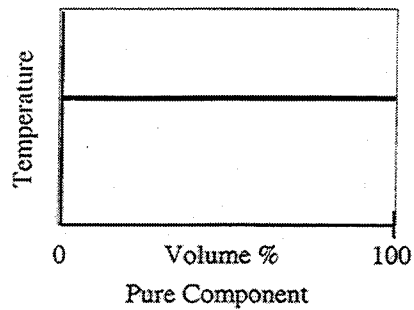
Properties Commonly Determined by Correlation

- True Boiling Point (TBP) distillation
- Average boiling points (VABP, MeABP, MABP, CABP)
- Molecular weight
- UOP K
- Cetane index
- Flowing gravity
- Heat capacity

VABP	—	Volume Average	Boiling	Point
MeABP	—	mean	"	"
MABP	—	Molal	"	"
CABP	—	Cubic	"	"

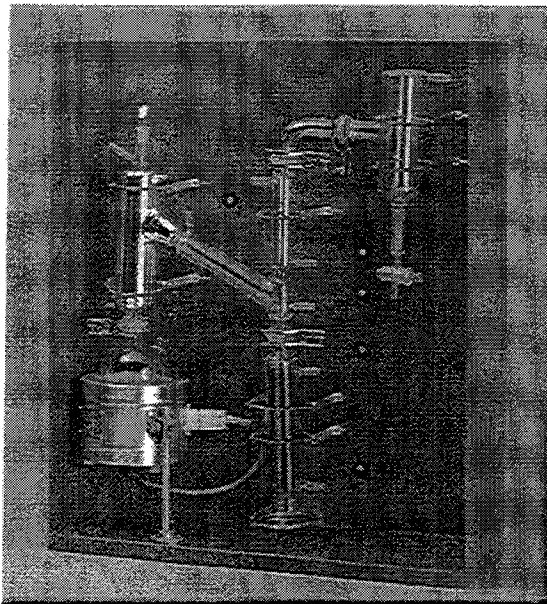
IPD-2004/HCP1-4

Boiling Point Curves



EDS-R00-1903
IPD-2004/HCP1-5

Laboratory Boiling Point Apparatus *ASTM D86 and D1160 Distillation*

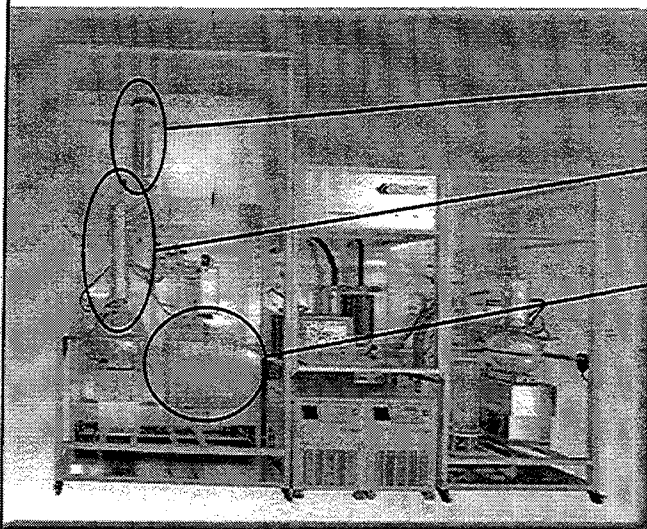


- No packing for separation
- Reflux results from heat loss in the neck of the flask
- Standardized
- D-86 is an atmospheric distillation
- D-1160 is a vacuum distillation, 1 - 50mmHg

IPD-R00-55
IPD-2004/HCP1-6

Laboratory Boiling Point Apparatus

ASTM D2892 (TBP) Distillation



- Reflux ratio of 5
- 15 to 20 theoretical stages
- Accurate component distribution for mixtures
- Requires greater sample volume, analysis time, expensive equipment

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ASTM - True Boiling Point Distillation Conversion

Example: Naphtha ASTM Distillation Conversion to TBP

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ASTM - True Boiling Point Distillation Conversion

Class Exercise: Crude Unit ASTM Distillation Conversion to TBP

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Types of Boiling Points

■ Volume Average Boiling Point

$$VABP = (T_{10} + T_{30} + T_{50} + T_{70} + T_{90}) / 5$$

■ Cubic Average Boiling Point

$$CABP = \left[\sum_{i=1}^n \left(\text{Volume Fraction} \times \sqrt[3]{bp(^{\circ}R)} \right) \right]^3$$

CABP is used to correlate UOP K, viscosity, and enthalpy

IPD-2004/HCP1-10

Types of Boiling Points

- Mean Average Boiling Point (MeABP)

$$MeABP = \frac{(CABP + MABP)}{2}$$

MeABP is used to correlate molecular weight and pseudo-critical pressure

IPD-2004/HCP1-11

Types of Boiling Points

- Molal Average Boiling Point (MABP)

$$MABP = \sum_{i=1}^n (\text{Mol Fraction} \times \text{Boiling Point})$$

MABP is used to correlate pseudo-critical temperature

- Weight Average Boiling Point (WABP)

$$WABP = \sum_{i=1}^n (\text{Weight Fraction} \times \text{Boiling Point})$$

WABP is used to correlate true critical temperature

IPD-2004/HCP1-12

Specific Gravity

SG^{T1/T2} means the fluid specific gravity at T1 relative to water at T2. For example,

$$^{\circ}\text{API} = 141.5 / \text{SG}^{60/60} - 131.5$$

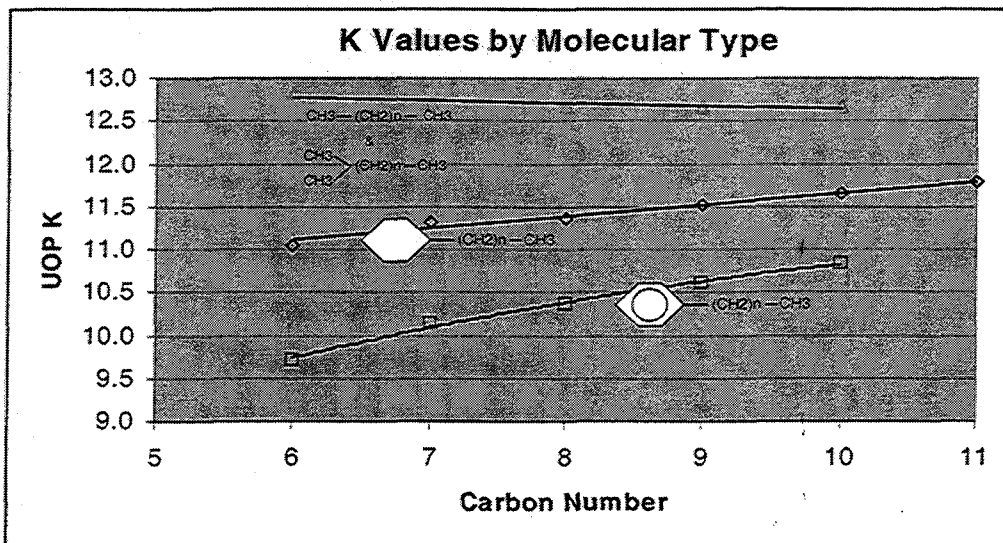
$$\text{SG}^{60/60} = 141.5 / (131.5 + ^{\circ}\text{API})$$

$$\text{SG water @ } 15.5^{\circ}\text{C} = 999.012\text{kg/m}^3$$

$$\text{SG water @ } 4.0^{\circ}\text{C} = 1000\text{kg/m}^3$$

IPD-2004/HCP1-13

UOP K Characterization Factor



IPD-2004/HCP1-14

UOP K Characterization Factor

Class Exercise: Calculate K Values of Three Different Intermediate Streams

IPD-2004/HCP1-15

UOP K Characterization Factor

$$\text{UOP K} = \frac{T^{1/3}}{\text{sp gr}} = \frac{(\text{CABP})^{1/3}}{\text{sp gr}}$$

$$\ln T^{1/3} = \ln \text{sp gr} + \ln K$$

$$\ln T = 3 \ln \text{sp gr} + 3 \ln K$$

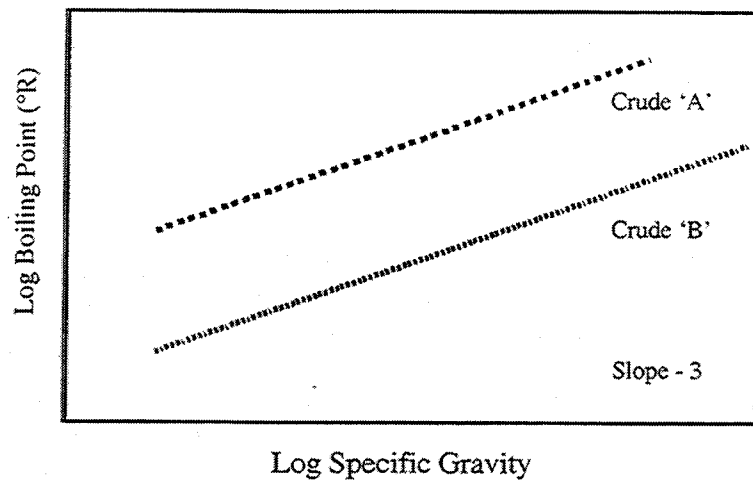
$$\ln T = 3 \ln \text{sp gr} + C$$

T = Cubic Average Boiling Point, °R

sp gr = Specific Gravity^{60°/60°}

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UOP K Characterization Factor



IPD-2004/HCP1-17

UOP K Characterization Factor

Class Exercise: Calculate K Value of A Crude Oil

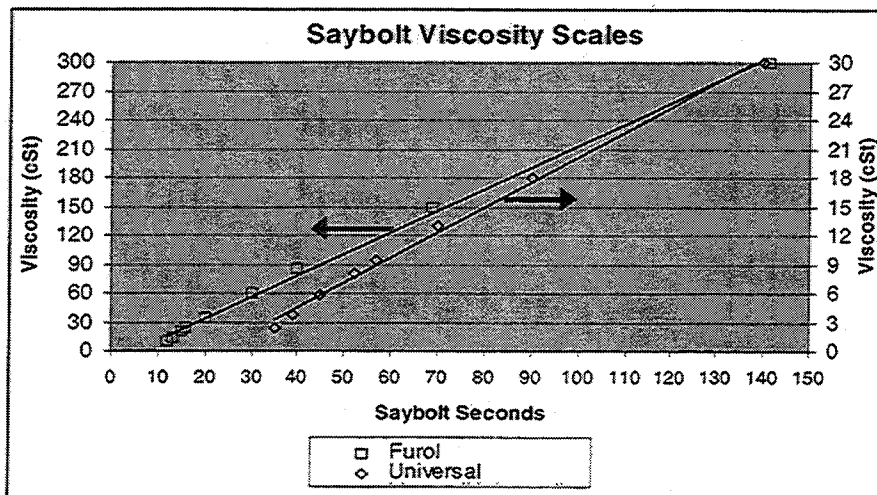
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Viscosity

- Viscosity characterize flow resistance
- Absolute Viscosity (μ) → Poise (g / cm-sec)
Centipoise = 0.01 * Poise
- $\nu = \mu / \rho$ ← *density at the temperature of viscosity measurement*
Kinematic Viscosity (ν) → Stokes (cm² / sec)
Centistoke (cSt) is more common

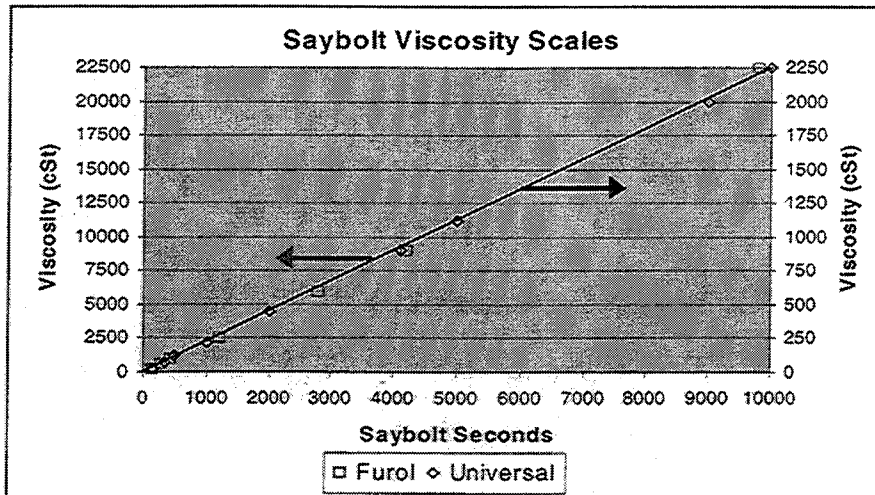
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Viscosity Interconversion of Saybolt Scales



IPD-2004/HCP1-20

Viscosity Interconversion of Saybolt Scales



IPD-2004/HCP1-21

Summary of Some Correlations

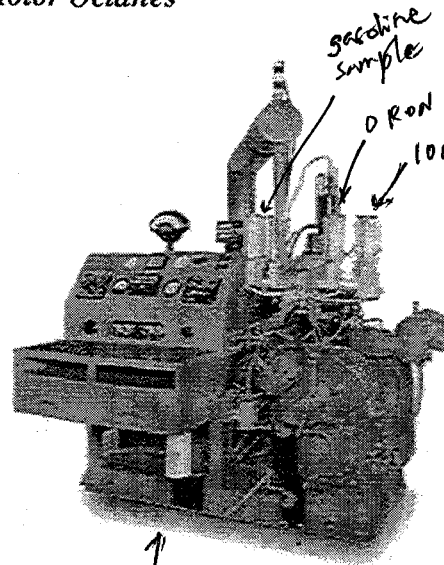
Method	Property	T 10%	T 50%	T 90%	SG	V 100°F (cSt)	V 210°F (cSt)	Volume Average Boiling Point	Distillation Slope	Mean Average Boiling Point	Cubic Average Boiling Point	UOP K
API 2B1.1	MeASP							X	X			
API 2B1.1	CASP							X	X			
API 2B1.1	MASP							X	X			
API 2B2.1	MW				X					X		
API 2B2.3	V 210°F (cSt)				X	X						
API 2B2.3	MW				X	X	X					
Definition	UOP K				X						X	
API 2B7.1	Flash Point	X										
ASTM D976	Cetane Index		X		X							
ASTM D4737	Cetane Index	X	X	X	X							
API 2B13.1	Cetane Index				X					X		
API 2B8.1	Pour Point				X					X		
API 2B8.1	Pour Point					X				X		
API 2B9.1	Aniline Point				X					X		X
API 2B10.1	Smoke Point									X		X
API 2B11.1	Freezing Point				X					X		X
API 2B12.1	Cloud Point				X					X		

IPD-2004/HCP1-22

Octane

Research and Motor Octanes

- Octane is a measure of a gasoline's resistance to pre-mature detonation in an engine.
- Pre-mature detonation is indicated by knocking.
- Octane is determined by burning gasoline in an engine under controlled conditions until a standard level of knocking occurs.
- The engine is next operated on a fuel blended from 2,2,4 trimethylpentane (100RON) and n- heptane (0 RON) that knocks at the same intensity as the gasoline sample.
- TEL is added to generate a standard higher than 100RON.
- Motor octane test simulates more severe engine operation.

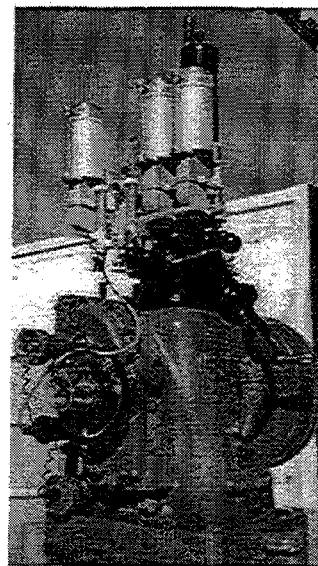


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Octane

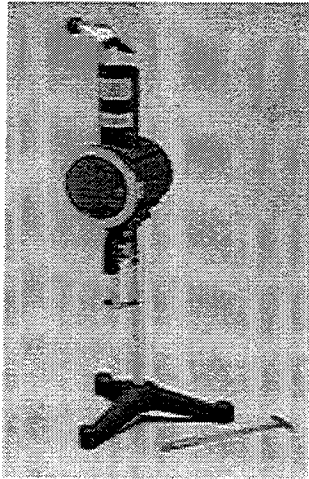
Research and Motor Octanes of Typical Gasoline Components

Blending Component	RON	MON
FCC Cracked Naphtha	91 - 93	-12
Reformate	95 - 103	-10
Alkylate	96 - 99	0
Isomerate	86 - 89	-1
Light Naphtha Hydrocrackate	76 - 78	-3
MTBE	118	-16
Toluene	110	-16
Ethanol	105	-14
n-Butane	93.8	-4



IPD-2004/HCP1-24

Smoke Point



- The maximum flame height achieved without smoking is the smoke point when tested in a standard wick-fed lamp
- Specification for Jet fuels and other kerosene products
- Some correlations for smoke point ...

ASTM :

$$SP \text{ (mm)} = 5.69 / [1.44 * SG + 0.00385 * A(lv\%) - 1]$$

API :

$$SP \text{ (mm)} = \exp[-1.028 + 0.474 * K - 0.00168 * MeABP(R)]$$

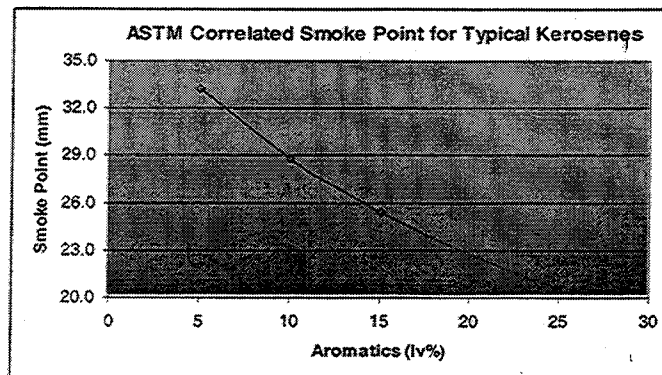
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Smoke Point

Aromatics Content (lv%)	Typical SG	ASTM Correlated Smoke Point (mm)
5	0.800	33.2
10	0.805	28.8
15	0.810	25.4
20	0.815	22.7
25	0.820	20.5

} Typical for kerosene hydrocrackate

} More typical for straight run kerosene

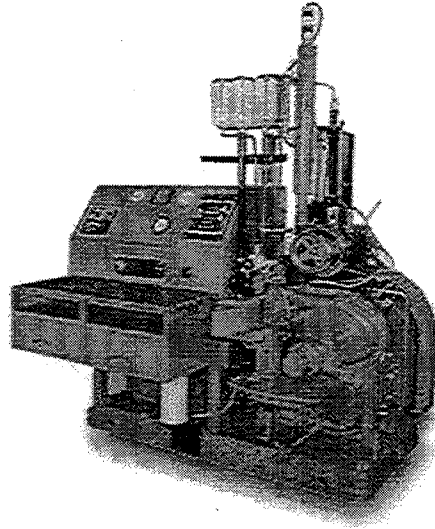


IPD-2004/HCP1-26

Cetane Number

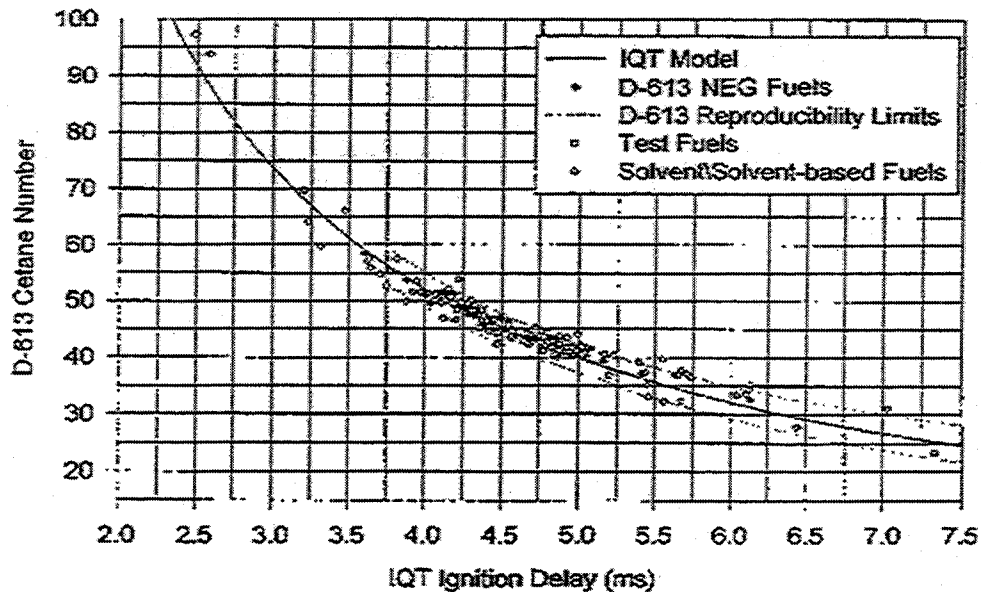
↑
C16

- Cetane number is a measure of ignition delay in a fuel's combustion
- Ignition delay is the time between the start of fuel injection and the start of fuel combustion
- Higher cetane number fuels will have shorter ignition delay periods than lower cetane number fuels
- Cetane number is determined from engine operation on a fuel blended from cetane (CN of 100) and α -methyl-naphthalene (CN of 0) that provides the same ignition quality to that of the test fuel.



IPD-2004/HCP1-27

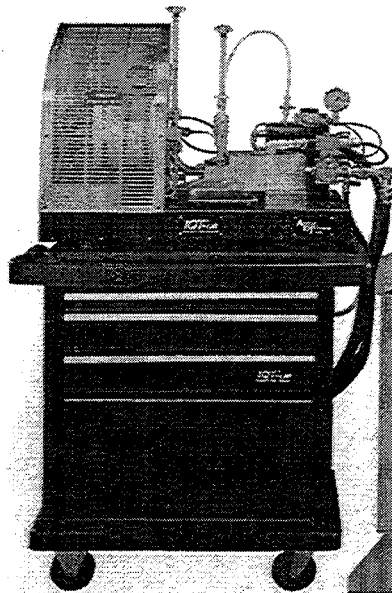
Cetane Number



IPD-2004/HCP1-28

Cetane Number

- Ignition delay technique incorporated for cetane measurement by Southwest Research Institute (SWRI)
- Measured cetane number is more accurate (± 1 CN) in comparison to CFR engine (± 3 CN)
- Being considered as an alternative to the cetane engine test method (ASTM D613)



IPD-2004/HCP1-29

Hydrocarbon	Boiling Point, °F	Cetane Number
Paraffins		
n-octane	259	63.8
n-decane	345	76.9
dodecane	421	87.6
tetradecane	489	96.1
cetane	549	100.0
octadecane	604	102.6
3-methylpentane	145	30.0
2,2,4-trimethylpentane	211	12.0
Olefins		
1-octene	252	40.5
1-decene	340	60.2
1-dodecene	415	71.3
1-tetradecene	261	82.7
1-hexadecene	525	84.2
1-octadecene	356	90.0
tetraisobutylene	464	4.5
Naphthenes		
butylcyclohexane	357	32.0
dicyclohexyl	462	47.4
decalin	367	42.1
cyclohexane	178	13.2
Aromatics		
benzene	177	0.0
toluene	231	-5.0
xylene		-10.0
metadiisopropylbenzene	399	-3.0
n-amyl benzene	399	18.0
n-hexyl benzene	439	32.0
n-heptyl benzene	464	39.0
n-nonylbenzene	536	50.0
n-dodecyl benzene	342	68.0
n-tetradecyl benzene	383	72.0
diphenyl	459	21.0
diphenylmethane	506	11.0
1,2-diphenylethane	545	1.0
α-methylnaphthalene	473	0.0

Cetane Number Cetane Number of Some Hydrocarbons

IPD-2004/HCP1-30



Training Services

Hydrocarbon Properties - Example of Naphtha ASTM Distillation Conversion

IPD-2004/HCP2-1

European Gasoline Specifications

Specification	2000	2005
Sulphur, mg/kg	150 max	50 max (10 max)*
RONC/MONC**	95 / 85 min	95 /85 min
Vapour pressure, kPa, summer	60 max	60 max
Distillation, % v/v @ 100°C	46 min	46 min
@ 150°C	75 min	75 min
Hydrocarbon analysis, % v/v		
Olefins	18 max	18 max
Aromatics	42 max	35 max
Benzene	1.0 max	1.0 max
Oxygen content, % m/m	2.7 max	2.7 max

* To be phased in between 2005 - 11

** Regular grade (91 / 81) not mentioned for 2005+

IPD-2004/HCP2-2

Options for Aromatics and Benzene Reduction in Future Gasoline Pool

- Dilution
 - Aromatics Extraction
 - Severity Reduction in Catalytic Reforming
 - Removal of Benzene Precursors
 - Benzene Destruction
- } Pre-fractionation
versus
Post-fractionation

IPD-2004/HCP2-3

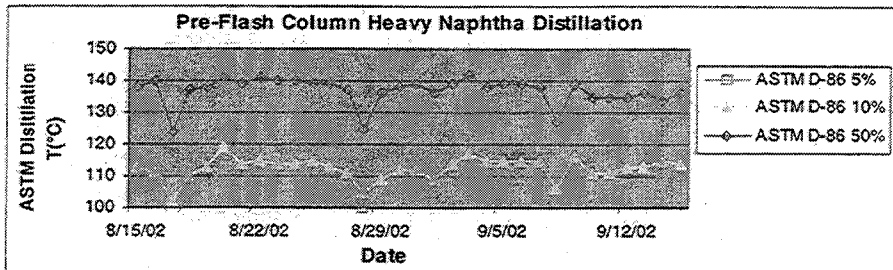
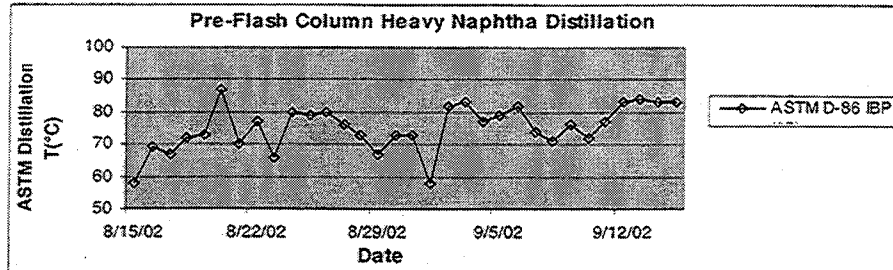
Benzene Precursors in Catalytic Reforming

Component	Normal Boiling Point (°C)
Methylcyclopentane	71.8
Benzene	80.1
Cyclohexane	80.7

- Catalytic reforming is a major contributor of benzene and aromatics in gasoline
- Benzene precursors quantitatively convert to benzene in reformate
- Removing benzene precursors in catalytic reforming feed by distillation is a “pre-fractionation” solution

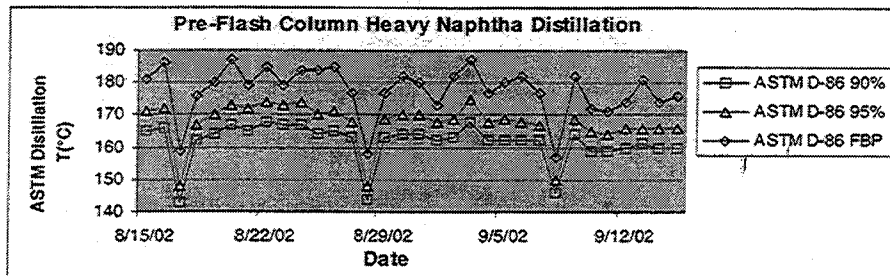
IPD-2004/HCP2-4

Preflash-Column Operation - Middle East Refiner **Conversion of ASTM Distillation to TBP**



IPD-2004/HCP2-5

Preflash-Column Operation - Middle East Refiner **Conversion of ASTM Distillation to TBP**



IPD-2004/HCP2-5

Preflash-Column Operation - Middle East Refiner *Conversion of ASTM Distillation to TBP*

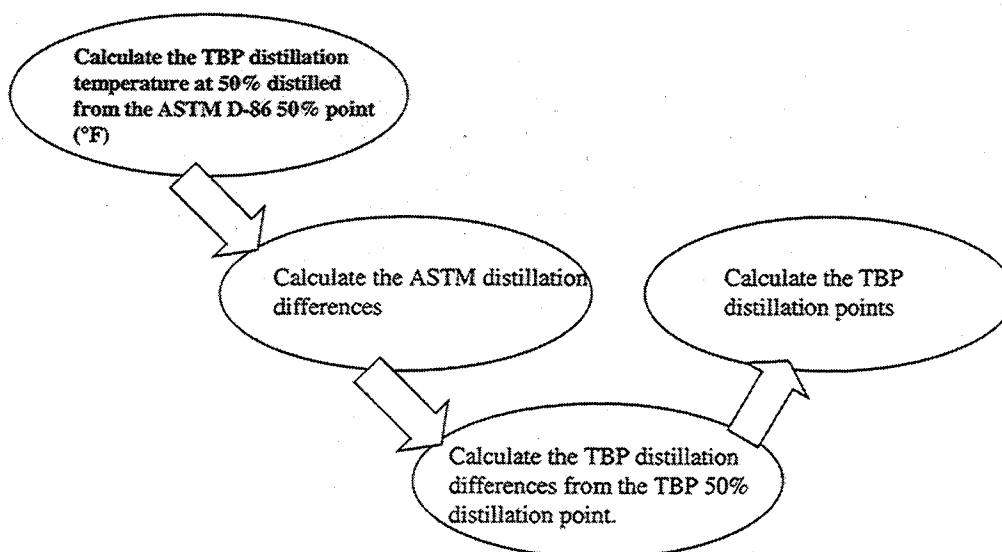
Initial
Boiling
Point →

ASTM Distillation Point	Heavy Naphtha Average Distillation (°C)	Heavy Naphtha Average Distillation (°F)	Heavy Naphtha Adjusted IBP (°C)	Heavy Naphtha Adjusted IBP (°F)
IBP	75	167	109	228
5%	107	224	119	245
10%	113	235	124	254
30%	126	258	132	269
50%	137	278	141	286
70%	148	298	152	305
90%	162	323	164	326
95%	167	333	170	337
FBP	178	352	178	352

- Convert the actual and adjusted distillation data to TBP distillations
- Does the actual column operation allow benzene precursors in feed? Does the adjusted operation exclude benzene precursors?

IPD-2004/HCP2-7

API Procedure 3A1.1 *ASTM D-86 Conversion to TBP*



IPD-2004/HCP2-8

API Procedure 3A1.1

50% TBP Distillation Point

$$\text{TBP (50)} = 0.8718 (\text{ASTM D-86(50)})^{1.0258}$$

$$\text{TBP (50)} = 0.8718 (278.3^{\circ}\text{F})^{1.0258}$$

$$\text{TBP (50)} = 280.5^{\circ}\text{F or } 138.1^{\circ}\text{C}$$

Let's use the actual average pre-flash column
naphtha as the example

IPD-2004/HCP2-9

API Procedure 3A1.1

Calculate ASTM Distillation Differences

ASTM Distillation Point	Heavy Naphtha Average Distillation (°F)	X _i
IBP	167	67
10%	235	24
30%	258	20
50%	278	0
70%	298	20
90%	323	24
FBP	352	29

Differences in interval

← 285 - 167
← 258 - 235

$$X_i = |\text{ASTM Distillation Point}_i - \text{ASTM Distillation Point}_{i-1}|$$

IPD-2004/HCP2-10

API Procedure 3A1.1

TBP Temperature Differences

constant

ASTM Distillation Point	i	A _i	B _i	X _i	Y _i
IBP	6	7.4012	0.60244	67	93
10%	5	4.9004	0.71644	24	47
30%	4	3.0306	0.80076	20	33
70%	3	2.5282	0.82002	20	30
90%	2	3.0419	0.75497	24	34
FBP	1	0.11798	1.6506	29	31

$$Y_i = A_i X_i^{B_i}$$

IPD-2004/HCP2-11

API Procedure 3A1.1

Calculate TBP Distillation Temperatures

$$\text{TBP (0)} = \text{TBP (10)} - Y_6$$

$$\text{TBP (10)} = \text{TBP (30)} - Y_5$$

$$\text{TBP (30)} = \text{TBP (50)} - Y_4$$

$$\text{TBP (70)} = \text{TBP (50)} + Y_3$$

$$\text{TBP (90)} = \text{TBP (70)} + Y_2$$

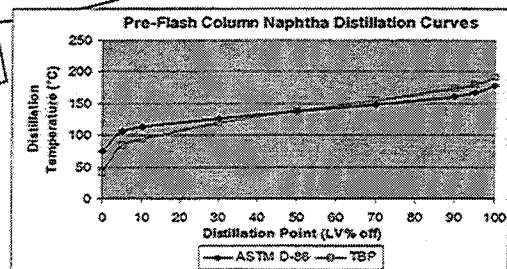
$$\text{TBP (100)} = \text{TBP (90)} + Y_1$$

IPD-2004/HCP2-12

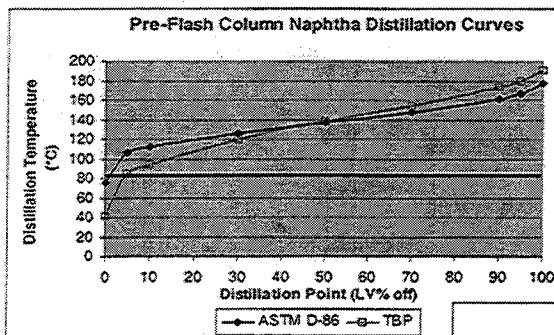
API Procedure 3A1.1

Calculate TBP Distillation Temperatures

Distillation Point	ASTM D-86 (°F)	TBP (°F)	ASTM D-86 (°C)	TBP (°C)
0	167	106	75	41
5	224	185	107	85
10	235	200	113	93
30	258	247	126	120
50	278	281	137	138
70	298	310	148	155
90	323	344	162	173
95	333	355	167	180
100	352	376	178	191



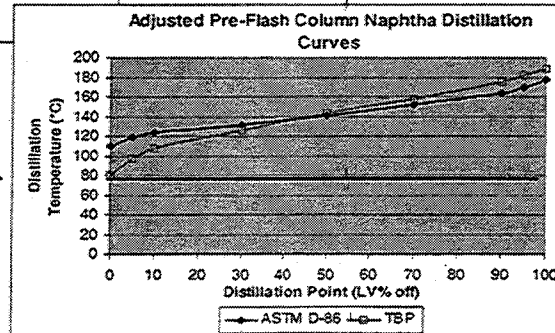
Pre-Fractionation for Benzene Precursor Reduction



Current distillation operation allows benzene precursors in feed

Proposed IBP adjustment mitigates benzene formation

IBP can be adjusted by increasing distillate rate/
reflux ratio





Training Services

Hydrocarbon Properties - Example of Determining Crude and Vacuum Unit TBP Cut Points

IPD-2004/HCP3-1

Test Run Data - Middle East Refiner

<u>STREAM</u>	<u>API</u> <u>(SP.GR.)</u>	<u>UOP K</u>	<u>m3/ d</u> <u>(m3/ h)</u>	<u>t/ d</u>	<u>vol %</u>	<u>wt. %</u>
Crude Charge	35.1	12.32	12908	10963	100	100
Vacuum Charge	19.3	11.66	6586	6180	51.0	56.4
Atm. Column Off Gas SG	(0.945)	---	(132)	4	0.1	0.0
Stabilizer Off Gas SG	(0.962)	---	(40)	1.1	0.0	0.0
Stab. O/ H Liquid LPG	117.2	---	171	97	1.3	0.9
LSRN	82.7	12.70	1000	660	7.7	6.0
HSRN	57.9	11.97	1687	1260	13.1	11.5
Kerosene	45.2	11.86	1591	1274	12.3	11.6
LAD	38.7	11.94	1286	1069	10.0	9.8
HAD	34.4	11.96	1007	859	7.8	7.8
Reduced Crude By-Pass	19.3	11.66	0	0	0.0	0.0
Stop Oil	40.4	13.27	52	43	0.4	0.4
LVGO	33.2	11.82	641	551	5.0	5.0
HVGO	26.2	12.12	2968	2663	23.0	24.3
Vacuum Residue	9.0	11.61	2665	2684	20.6	24.5
Recovery			13068	11166	101.4	101.8

IPD-2004/HCP3-2

Test Run Data - Middle East Refiner

LABORATORY TEST RESULTS

Stream	LSRN	HSRN	KERO	LAD	HAD	LVGO	HVGO
Saybolt Color	+30	+30	+30	---	---	---	---
ASTM Color	---	---	---	---	---	<1	4.50
ASTM Distillation (°C)							
IBP	31	91	156	214	251	268	327
5 %	34	106	170	237	268	280	374
10 %	36	108	175	244	275	284	391
30 %	44	115	189	253	296	297	419
50 %	54	122	202	267	313	309	444
70 %	68	135	221	288	343	324	474
90 %	82	148	240	309	373	339	504
95 %	94	158	252	321	393	348	523
EP	103	173	266	343	400	365	550
Flash Point (°C, PM)	---	---	46	77	113	128	---
Pour Point (°C)	---	---	---	-18	-6	-6	---
RVP (psi)	16.5	---	---	---	---	---	---
GAP	12	12	-15	-53	---	---	---

IPD-2004/HCP3-3

ASTM to TBP Conversion Worksheet

ASTM Distillation		ASTM ΔT	TBP ΔT	TBP Distillation	
IBP					IBP
10%					10%
30%					30%
50%					50%
70%					70%
90%					90%
FBP					FBP

IPD-2004/HCP3-4

Test Run Data - Middle East Refiner

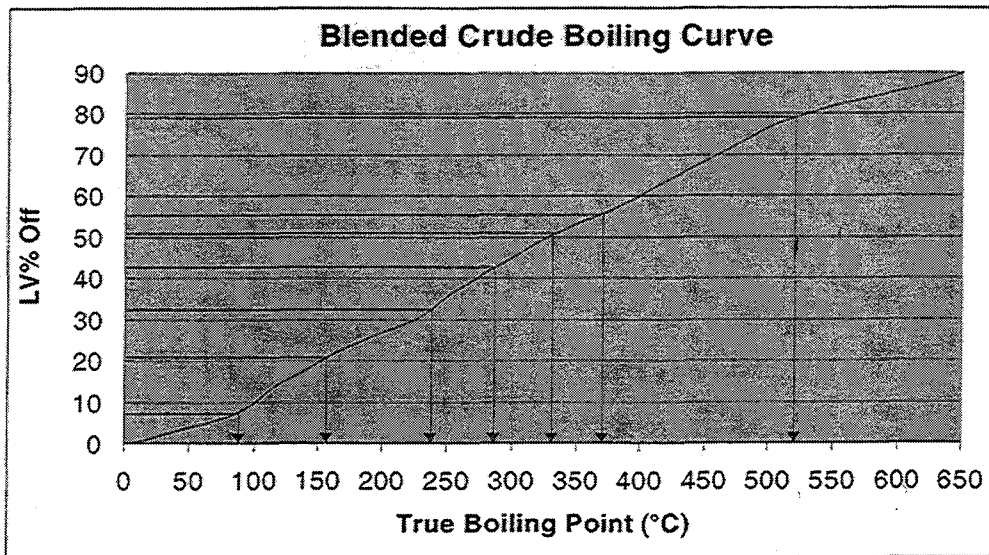
Conversion of ASTM Distillations to TBP

Stream	LSRN	HSRN	Kero	Light Diesel	Heavy Diesel	LVGO	HVGO	VR
TBP Distillation								
IBP	4	61	121	182	218	240	302	487
5%	11	88	146	218	246	283	360	519
10%	16	92	155	229	258	270	382	542
20%	23	101	168	240	276	283	401	
30%	32	107	181	247	292	295	414	
40%	40	112	191	257	305	305	429	
50%	49	119	202	270	319	315	444	
60%	60	129	215	284	337	326	459	
70%	70	139	229	299	358	337	474	
80%	79	147	241	312	376	346	488	
90%	89	157	254	326	393	357	504	
95%	103	168	267	339	415	367	523	
100%	113	184	282	363	423	386	550	750

IPD-2004/HCP3-5

Test Run Blended Crude

Liquid - Volume



IPD-2004/HCP3-6

Test Run Crude Cut Points

Cut Point	Value (°C)
Light Naphtha - Heavy Naphtha	89
Heavy Naphtha - Kerosene	158
Kerosene - Light Diesel	240
Light Diesel - Heavy Diesel	289
Heavy Diesel - LVGO	336
LVGO - HVGO	374
HVGO - Vacuum Residue	523



Training Services

Hydrocarbon Properties - Example of Calculating UOP K Values

IPD-2004/HCP4-1

Three Very Different Intermediates

Stream	120VI Lube Basestock	Highly Saturated FCC LCO	102RON Heavy Reformate
Source	U.S. Refiner	Pilot Plant	UOP Reactor Model
SG	0.8639	0.8550	0.8441
Distillation Method	D-1100	D-60	D-86
IBP (°C)	430.0		110.6
5%	441.7		117.2
10%	444.4	173.9	121.7
30%	453.9	216.1	132.2
50%	460.6	234.4	144.4
70%	472.8	250.0	160.0
90%	497.8	282.2	168.2
95%	506.1		181.1
FBP	602.2		194.4
S (wt%)	0.0014	0.0058	0
Total N (wppm)	2	1.2	0

Similar specific
gravity

However, distillations are in
VGO, distillate and naphtha
ranges

IPD-2004/HCP4-2

Calculation of UOP K Value

Calculate VABP

Calculate distillation slope

Calculate temperature correction; determine CABP

Calculate K from CABP and SG

IPD-2004/HCP4-3

Three Very Different Intermediates Calculate Volume Average Boiling Point

Stream	120VI Lube Basestock	Highly Saturated FCC LCO	102RON Heavy Reformate
Source	U.S. Refiner	Pilot Plant	UOP Reactor Model
SG	0.8639	0.8550	0.8441
Distillation Method	D-1160	D-86	D-86
IBP (°C)	430.0		110.6
5%	441.7		117.2
10%	444.4	173.9	121.7
30%	453.9	216.1	132.2
50%	460.6	234.4	144.4
70%	472.8	250.0	160.0
90%	497.8	282.2	169.4
95%	506.1		181.1
FBP	602.2		194.4
S (wt%)	0.0014	0.0058	0
Total N (wppm)	2	1.2	0

$$\bullet \text{ VABP} = (T_{10} + T_{30} + T_{50} + T_{70} + T_{90}) / 5$$

$$\bullet \text{ VABP (°C)} = (444 + 454 + 461 + 473 + 498) / 5 = 467^{\circ}\text{C}$$

$$\text{VABP (°F)} = 872^{\circ}\text{F}$$

IPD-2004/HCP4-4

Three Very Different Intermediates Calculate Distillation Slope

Stream	120VI Lube Basestock	Highly Saturated FCC LCO	102RON Heavy Reformate
Source	U.S. Refiner	Pilot Plant	UOP Reactor Model
SG	0.8639	0.8550	0.8441
Distillation Method	D-1160	D-88	D-86
IBP (°C)	430.0		110.6
5%	441.7		117.2
10%	444.4	173.9	121.7
30%	456.9	216.1	132.2
50%	460.6	234.4	144.4
70%	472.8	250.0	160.0
90%	497.8	282.2	169.4
95%	506.1		181.1
FBP	602.2		194.4
S (wt%)	0.0014	0.0058	0
Total N (wppm)	2	1.2	0

- Slope = $(T_{90} - T_{10}) / 80$
- Slope = $(498 - 444) / 80 = 0.675 \text{ } ^\circ\text{C}/\%$
Slope = $1.215 \text{ } ^\circ\text{F}/\%$

IPD-2004/HCP4-5

Three Very Different Intermediates Calculate Temperature Correction to VABP

- $\text{CABP} = \text{VABP} - \Delta_3 \text{ (API 2B1.1-3)}$
- $\ln \Delta_3 = -0.23589 - 0.06906 * (\text{VABP} - 32)^{0.45} + 1.8858 * \text{Slope}^{0.45} \text{ (API 2B1.1-7)}$
- VABP and distillation slope are in units of $^\circ\text{F}$ and $^\circ\text{F}/\%$
- $\Delta_3 = 1.5^\circ\text{F}$
- $\text{CABP} = 872 - 1.5 = 870^\circ\text{F}$ (or 1330R)
- $\text{UOP K} = (1330\text{R})^{1/3} / 0.864 = 12.73$

$\Delta_3 = e^{(\dots)}$
 $\Rightarrow \text{in excel} = \text{EXP}(\dots)$

IPD-2004/HCP4-6

Three Very Different Intermediates

Class Exercise

Stream	120VI Lube Basestock	Highly Saturated FCC LCO	102RON Heavy Reformate
Source	U.S. Refiner	Pilot Plant	UOP Reactor Model
SG	0.8639	0.8550	0.8441
Distillation Method	D-1160	D-86	D-86
IBP (°C)	430.0		110.6
5%	441.7		117.2
10%	444.4	173.9	121.7
30%	453.9	216.1	132.2
50%	460.6	234.4	144.4
70%	472.8	250.0	160.0
90%	497.8	282.2	169.4
95%	506.1		181.1
FBP	602.2		194.4
S (wt%)	0.0014	0.0058	0
Total N (wppm)	2	1.2	0
VABP (C): API 2-0.3	465.9		
(F)	870.6		
Slope (F%): API 2B.1	1.20		
Correction for CABP (F): API 2B1.1-7	1.5		
CABP (R): API 2B1.1-3	1328.8		
UOP K (SG, Distillation)	12.73		

IPD-2004/HCP4-7

Three Very Different Intermediates

Class Exercise

Stream	120VI Lube Basestock	Highly Saturated FCC LCO	102RON Heavy Reformate
Source	U.S. Refiner	Pilot Plant	UOP Reactor Model
SG	0.8639	0.8550	0.8441
Distillation Method	D-1160	D-86	D-86
IBP (°C)	430.0		110.6
5%	441.7		117.2
10%	444.4	173.9	121.7
30%	453.9	216.1	132.2
50%	460.6	234.4	144.4
70%	472.8	250.0	160.0
90%	497.8	282.2	169.4
95%	506.1		181.1
FBP	602.2		194.4
S (wt%)	0.0014	0.0058	0
Total N (wppm)	2	1.2	0
VABP (C): API 2-0.3	465.9	231.3	145.6
(F)	870.6	448.4	294.0
Slope (F%): API 2B.1	1.20	2.44	1.08
Correction for CABP (F): API 2B1.1-7	1.5	4.7	2.4
CABP (R): API 2B1.1-3	1328.8	903.4	751.3
UOP K (SG, Distillation)	12.73	11.31	10.77
Paraffin Content (lv%)	65	18	22
Naphthene Content (lv%)	30	56	0
Aromatics Content (lv%)	4	16	78

UOP K
Paraffins 12-13
Naphthenes 11-12
Aromatics 10-11

IPD-2004/HCP4-8



Training Services

Hydrocarbon Properties - Example of Determining Crude K Value

IPD-2004/HCP5-1

Test Run Data - Middle East Refiner

<u>STREAM</u>	<u>API</u> <u>(SP.GR.)</u>	<u>UOP K</u>	<u>m³ / d</u> <u>(m³ / h)</u>	<u>t / d</u>	<u>vol %</u>	<u>wt. %</u>
Crude Charge	35.1	12.32	12908	10963	100	100
Vacuum Charge	19.3	11.66	6586	6180	51.0	56.4
Atm. Column Off Gas SG	(0.945)	---	(132)	4	0.1	0.0
Stabilizer Off Gas SG	(0.962)	---	(40)	1.1	0.0	0.0
Stab. O / H Liquid LPG	117.2	---	171	97	1.3	0.9
LSRN	82.7	12.70	1000	660	7.7	6.0
HSRN	57.9	11.97	1687	1260	13.1	11.5
Kerosene	45.2	11.86	1591	1274	12.3	11.6
LAD	38.7	11.94	1286	1069	10.0	9.8
HAD	34.4	11.96	1007	859	7.8	7.8
Reduced Crude By-Pass	19.3	11.66	0	0	0.0	0.0
Slop Oil	40.4	13.27	52	43	0.4	0.4
LVGO	33.2	11.82	641	551	5.0	5.0
HVGO	26.2	12.12	2968	2663	23.0	24.3
Vacuum Residue	9.0	11.61	2665	2684	20.6	24.5
Recovery			13068	11166	101.4	101.8

IPD-2004/HCP5-2

Test Run Data - Middle East Refiner

LABORATORY TEST RESULTS

Stream	LSRN	HSRN	KERO	LAD	HAD	LVGO	HVGO
Saybolt Color	+30	+30	+30	---	---	---	---
ASTM Color	---	---	---	---	---	<1	4.50
ASTM Distillation (°C)							
IBP	31	91	156	214	251	268	327
5 %	34	106	170	237	268	280	374
10 %	36	108	175	244	275	284	391
30 %	44	115	189	253	296	297	419
50 %	54	122	202	267	313	309	444
70 %	68	135	221	288	343	324	474
90 %	82	148	240	309	373	339	504
95 %	94	158	252	321	393	348	523
EP	103	173	266	343	400	365	550
Flash Point (°C, PM)	---	---	46	77	113	128	---
Pour Point (°C)	---	---	---	-18	-6	-6	---
RVP (psi)	16.5	---	---	---	---	---	---
GAP	12	12	-15	-53	---	---	---

IPD-2004/HCP5-3

Test Run Data - Middle East Refiner

Calculate Cubic Average Boiling Points of Individual Cuts

Answer:

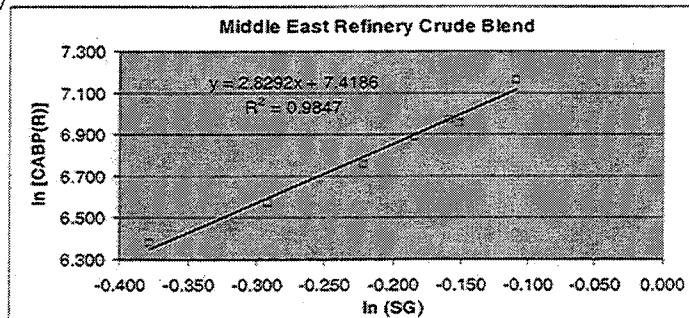
Cut	CABP (°F)
Light Naphtha	131
Heavy Naphtha	258
Kerosene	401
Light Diesel	521
Heavy Diesel	607
LVGO	590
HVGO	835

IPD-2004/HCP5-4

Test Run Data - Middle East Refiner

Plot CABP v. SG on Log Basis

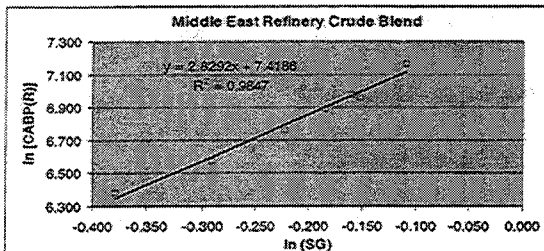
Cut	SG	CABP (°F)	ln SG	ln CABP(R)
Light Naphtha	0.685	131	-0.378	6.382
Heavy Naphtha	0.747	258	-0.292	6.576
Kerosene	0.801	401	-0.222	6.758
Light Diesel	0.831	521	-0.185	6.889
Heavy Diesel	0.853	607	-0.159	6.973
LVGO	0.859	590	-0.152	6.957
HVGO	0.897	835	-0.108	7.166



IPD-2004/HCP5-5

Test Run Data - Middle East Refiner

Analysis of K Value Plot



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.992
R Square	0.985
Adjusted R Squ	0.982
Standard Error	0.036
Observations	7

Slope is statistically equal to 3

	Coefficients	Standard Error	Lower 95%	Upper 95%
Intercept	7.41860532	0.03635237	7.32516	7.512053126
X Variable 1	2.82921471	0.15786734	2.423559	3.234870348

- Intercept is 7.419
- Intercept = C
- $C / 3 = \ln K$
- $K_{\text{crude}} = 11.85$

IPD-2004/HCP5-6

Octane is a figure of merit representing the resistance of gasoline to premature detonation when exposed to heat and pressure in the combustion chamber of an internal-combustion engine. Such detonation is wasteful of the energy in the fuel and potentially damaging to the engine; premature detonation is indicated by knocking or pinging noises that occur as the engine operates. If an engine running on a particular gasoline makes such noises, they can be lessened or eliminated by using a gasoline with a higher octane number. The octane number of a sample of fuel is determined by burning the gasoline in an engine under controlled conditions, e.g., of spark timing, compression, engine speed, and load, until a standard level of knock occurs. The engine is next operated on a fuel blended from a form of isooctane that is very resistant to knocking and a form of heptane that knocks very easily. When a blend is found that duplicates the knocking intensity of the sample under test, the percentage of isooctane by volume in the blended sample is taken as the octane number of the fuel. Octane numbers higher than 100 are found by measuring the amount of tetraethyl lead that must be added to pure isooctane to duplicate the knocking of a sample fuel. At present three systems of octane rating are used in the United States. Two of these, the research octane and motor octane numbers, are determined by burning the gasoline in an engine under different, but specified, conditions. Usually the motor octane number is lower than the research octane. The third octane rating, which federal regulations require on commercial gasoline pumps, is an average of research octane and motor octane. Under this system a regular grade gasoline has an octane number of about 87 and a premium grade of about 93. Most American-made cars that were built in the 1971 model year or later can use regular gasoline. To prevent knocking, premium grade gasoline must be used in many cars built before 1971 and in some new cars that have high-performance engines.

For clarity it is useful to provide a general overview of an octane number. An octane number is a quantitative, but imprecise measure of the maximum compression ratio at which a particular fuel can be utilized in an engine without some of the fuel/air mixture "knocking" or self igniting. This self ignition of the air/fuel mixture in the cylinder results in a loss of peak power. Directionally as the compression ratio of the engine increases so does the required octane number of the gasoline if engine knocking is to be avoided.

The performance of an engine is dependent upon many factors, one of which is the severity of operation. Accordingly the performance of a fuel is also dependent upon engine severity. To account for differences in the performance quality of a fuel two engine octane numbers are routinely used. The Research Octane Number (RON, or F1) simulates fuel performance under low severity engine operation. The Motor Octane Number (MON, or F2) simulates more severe operation that might be incurred at high speed or high load. In practice the octane of a gasoline is reported as the average of RON and MON or $R+M/2$.

Classically, both numbers are measured with a standardized single cylinder, variable compression ratio engine. For both RON and MON, the engine is operated at a constant speed (RPM's) and the compression ratio is increased until the onset of knocking. For RON engine speed is set at 600 rpm and MON is at 900 rpm.

explosion
Octane is a rating of a fuel's resistance to ignite. The higher the octane, the harder it is to get to ignite. A higher octane may be necessary to prevent pre-ignition and detonation in a high performance engine. Higher octane fuel will generally burn slightly slower than a lower octane fuel which could require a change in ignition timing. Using more octane than you need will not help power, the slower burn rate will actually cause you to lose some power.

Detonation

Normal combustion will take place at a pretty steady rate (for a given rpm and load), when a large amount of the charge burns extremely fast and uncontrollably, it is known as detonation. Detonation can destroy an engine in a matter of seconds. It is common knowledge that heat causes detonation, but heat is not the only cause. Pressure plays a big role in it also. You can get detonation by running with too much ignition advance, if heat was the only cause, signs of detonation would be around the exhaust valve, but this is not the case. Usually when detonation takes place from too much advance, the detonation occurs on the intake side of the chamber, which is the coolest side of the chamber. This happens because detonation did not occur until the pressure got excessive, which was after the spark. By the time that happened, the charge near the exhaust valve has already been burned. Most of the time, detonation will occur after normal combustion has started. Apart from destroying pistons and spark plugs, light detonation can cause all sorts of other problems, like fatiguing cranks and rods quickly and pounding bearings to death, so avoid detonation at all costs.

Pre-Ignition

When the charge lights off before the spark, it's called pre-ignition. This can happen with or without detonation, but usually will cause detonation in a high performance engine. Hot spots in the combustion chamber are the usual cause of pre-ignition. A spark plug with a high heat range can cause a hot spot. When pre-ignition occurs, the charge begins to burn, then when the spark plug sparks there are two flame fronts. This is very unpredictable and can lead to detonation, because it will act just like too much ignition timing, but it won't be controllable.

Motor Octane Rating

The motor octane rating, referred to as MON (motor octane number), is the best rating to use when selecting fuel for your race or high compression engine. When testing MON, the fuel is heated to 300° F and the intake air is heated to 100° F. The test engine is a single cylinder 4 cycle engine that is run at 900 rpm. Ignition timing is varied with compression ratio. Engine load is varied during test.

Research Octane Rating

Known as RON (research octane rating). Tested at 600 rpm with a fixed timing of 13° BTDC. The fuel temp is not controlled at all and the intake air temp is varied with barometric pressure. This is done to convert everything to a SAE standard day, which is 60° F, 0% Humidity, and 29.92 inches barometric pressure. The RON should not be used when selecting fuel for a race or high performance engine. The RON will always be higher than the MON.

The Importance of Cetane Number in Diesel Fuel

What is Cetane Number?

- **Cetane Number is a measure of the ignition quality of a diesel fuel.** It is often mistaken as a measure of fuel quality. Cetane number is actually a measure of a fuel's ignition delay. This is the time period between the start of injection and start of combustion (ignition) of the fuel. In a particular diesel engine, higher cetane fuels will have shorter ignition delay periods than lower cetane fuels.
- **Cetane number should not be considered alone when evaluating diesel fuel quality.** API gravity, BTU content, distillation range, sulfur content, stability and flash point are also very important. In colder weather, cloud point and low temperature filter plugging point may be critical factors.

CETANE NUMBER – ANOTHER DEFINITION

The most accurate method of assessing the ignition quality of a diesel fuel is by measuring its cetane number in a test engine, the higher the cetane number the higher the ignition quality. The cetane number of a fuel is defined as the percentage of cetane, arbitrarily given a cetane number of 100, in a blend with alphamethyl-naphthalene (cetane number -0), which is equivalent in ignition quality to that of the test fuel.

Determining Cetane Number

- **The optical method for determining cetane number is ASTM test D-613.** This method requires the use of an industry standard test engine equipped with accepted instrumentation and operated under specific conditions. In this test, the engine compression ratio is varied for the test sample and reference fuels of known cetane number to obtain a fixed ignition delay. The compression ratio of the sample is bracketed by those of two reference fuels. The cetane number of the sample fuel is determined by estimating between the two reference fuel points.
- **Because the ASTM D-613 test is time consuming and expensive, calculated cetane index (ASTM D-976 or D-4737 is often substituted for cetane number.** The calculated cetane index is derived from the fuel's density and boiling range. While useful for estimating the cetane number of distillate fuels, this technique can not be applied to fuels containing additives that raise cetane number. These additives do not change the fuel density or distillation profile, so they do not alter the calculated cetane index.

How Does Cetane Number Affect Engine Operation?

- **There is no benefit to using a higher cetane number fuel than is specified by the engine's manufacturer.** The ASTM Standard Specification for Diesel Fuel Oils (D-975) states, "The cetane number requirements depend on engine design, size, nature of speed and load variations, and on starting and atmospheric conditions. Increase in cetane number over values actually required does not materially improve engine performance. Accordingly, the cetane number specified should be as low as possible to insure maximum fuel availability." This quote underscores the importance of matching engine cetane requirements with fuel cetane number.
- **Diesel fuels with cetane number lower than minimum engine requirements can cause rough engine operation.** They are more difficult to start, especially in cold weather or at high altitudes. They accelerate lube oil sludge formation. Many low cetane fuels increase engine deposits resulting in more smoke, increased exhaust emissions and greater engine wear.
- **Using fuels which meet engine operating requirements will improve cold starting, reduce smoke during start-up, improve fuel economy, reduce exhaust emissions, improve engine durability and reduce noise and vibration.** These engine fuel requirements are published in the operating manual for each specific engine or vehicle.

- **Overall fuel quality and performance depend on the ratio of paraffinic and aromatic hydrocarbons**, the presence of sulfur, water, bacteria, and other contaminants, and the fuel's resistance to oxidation. The most important measures of fuel quality include API gravity, heat value (BTU content), distillation range and viscosity. Cleanliness and corrosion resistance are also important. For use in cold weather, cloud point and low temperature filter plugging point must receive serious consideration. Cetane number does not measure any of these characteristics.

Cetane Improvers / Ignition Accelerators

- **U S diesel fuels are blends of distillate fuels and cracked petroleum hydrocarbons.** The cracked hydrocarbons are low cetane compounds, largely due to their aromatic content. To meet the cetane number demands of most diesel engines, cetane improvers must be added to these blends. The lower cetane cracked compounds are less responsive to these cetane improvers than the higher cetane paraffinic fuels.
- **Cetane improvers modify combustion in the engine.** They encourage early and uniform ignition of the fuel. They discourage premature combustion and excessive rate of pressure increase in the combustion cycle. Depending on the amount of high versus low cetane components in the base fuel, typical alkyl nitrate additive treatments can increase cetane by about 3 to 5 numbers (1:1000 ratio). With high natural cetane premium base fuels (containing a high percentage of paraffins) and a 1:500 treatment ratio, cetane may increase up to a maximum of about 7 numbers.
- **Most cetane improvers contain alkyl nitrates** which break down readily to provide additional oxygen for better combustion. They also break down and oxidize fuel in storage. This generates organic particulates, water, and sludge - all of which degrade fuel quality. The result is often a fuel which no longer meets even minimum requirements. Because of these drawbacks, nitrate cetane improvers are not used in DurAlt fuel conditioners.
- **DurAlt fuel conditioners** are blended to improve oxidation stability, while providing a cetane number increase of 2 to 5 numbers. DurAlt products are designed to improve combustion while reducing oxidation and particulate formation, increasing storage stability, and enhancing fuel quality.

Do Cetane Improving Additives Really Improve Fuel Quality?

- **Fuel quality is defined** by the physical property specifications given in the ASTM Standard Specification for Diesel Fuel Oils, ASTM D-975. Carbon residue, ash and sulfur increase engine wear and deposit formation. Premium diesel fuels should have lower specifications for these properties. Additionally, premium diesel fuels should be more stable in storage than standard fuels, so the premium fuel quality you purchase won't degrade over time. This is the area where nitrate-containing cetane improvers cause problems.
- **More fuel retailers are introducing premium diesel fuels, touting high cetane number as the sole benchmark of fuel quality.** Contrary to this assumption, a cetane number which is too high may cause too short an ignition delay period. This changes the timing of the pressure peak, resulting in loss of power. When this happens, many of the performance problems associated with low cetane fuel will result. While the problems due to low cetane largely disappear after the engine warms up, with too high a cetane, these problems will persist even with a hot engine.

Specifying Diesel Fuel

Cetane number is an important measure of ignition quality, or cold-starting ability. API gravity is an excellent indicator of heat value, which translates into fuel economy and power. The distillation curve reflects the molecular weight distribution, with higher boiling fractions providing better lubrication, higher cetane - and more deposits. Sulfur content is directly related to corrosion; this needs to be as low as possible. Oxidation stability, water, and sediment content affect the storage life of the oil. For winter use, low cloud point and low temperature filter plugging point are critical to uninterrupted operation. To insure the best quality fuel for your diesel engines, follow the engine manufacturer's specifications for all these characteristics